Reconstruction and Computing Techniques inspired by Deep Learning

Amir Farbin
University of Texas Arlington

Deep Learning

- A brief introduction... assuming you are familiar with Neutral Networks
- Disclaimer: I'm not a Deep Learning expert...
 - I'm borrowing slides from others (mostly from the <u>Data Science @ LHC Workshop</u>)
- What is it? I guess technically, multi (many?) layer Neural Networks with large number of parameters.
- Why now? Difficulty training such big networks in the past.
 - Solutions to difficulties in training (e.g. vanishing gradient problem)
 - Big Data provides the necessary large datasets for training
 - GPUs
- Why is deep better than shallow?
 - Eliminate Feature Engineering
 - For shallow networks, most if *your* time spent on... developing algorithms that process raw data into the inputs to the NN.
 - Deep NNs can learn features from raw data. Save you time, and possibly the DNN learn features that are better than anything you could have come up with.
 - Unsupervised learning: DNNs classify events without being told what are the classes. The hope is that they could make sense of complicated data which we don't understand.

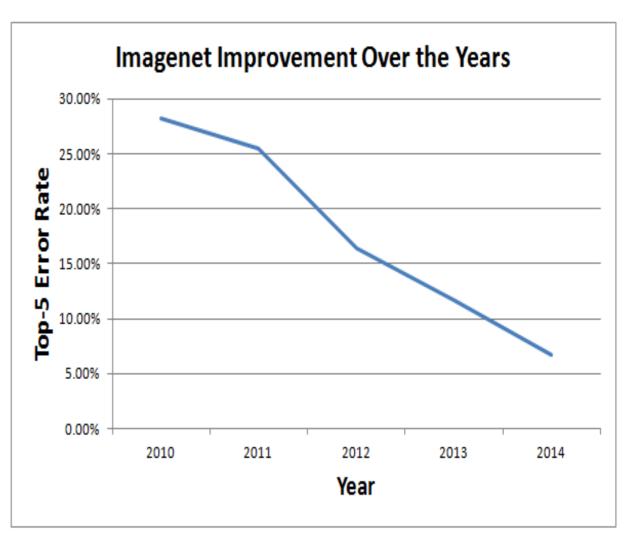
Recent History

- Deep Learning feats that sparked broad interest:
 - 2012, Google 1B DNN learns to identify cats (and 20000 other types of objects) (Wired Article, paper)
 - No features: trained with 200x200 pixel images from YouTube
 - Unsupervised: the pictures were unlabeled.
 - Google cluster 16000 cores ~ \$1M. Redone with \$20k system with GPUs.
 - 2013: Deep Mind builds AI that plays ATARI (<u>Blogpost</u>, <u>Nature, YouTube</u>)

Computer Vision - Image Classification

Imagenet

- Over 1 million images, 1000 classes, different sizes, avg 482x415, color
- 16.42% Deep CNN dropout in 2012
- 6.66% 22 layer CNN (GoogLeNet) in 2014
- 4.9% (Google, Microsoft) superhuman performance in 2015



Sources: Krizhevsky et al ImageNet Classification with Deep Convolutional Neural Networks, Lee et al Deeply supervised nets 2014, Szegedy et al, Going Deeper with convolutions, ILSVRC2014, Sanchez & Perronnin CVPR 2011, http://www.clarifai.com/Benenson, http://rodrigob.github.io/are_we_there_yet/build/classification_datasets_results.html

Examples























Input Output Pixels: "ear" Audio: "sh ang hai res taur aun ts" <query, doc1, doc2> P(doc1 preferred over doc2) "Hello, how are you?" "Bonjour, comment allez-vous?"

Good Generalization





Both recognized as a "meal"

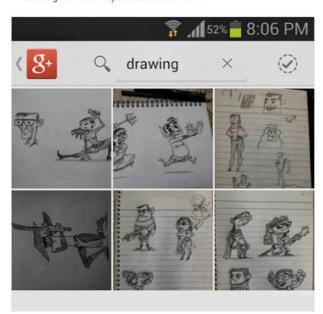
Good Fine-grained Classification

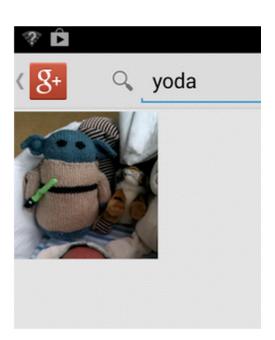


"hibiscus"

"dahlia"

Google Plus photo search is awesome. Searched with keyword 'Drawing' to find all my scribbles at once:D







Generating Image Captions from Pixels





Human: A young girl asleep on the sofa cuddling a stuffed bear.

Model sample 1: A close up of a child holding a stuffed animal.

Model sample 2: A baby is asleep next to a teddy bear.

Generating Image Captions from Pixels

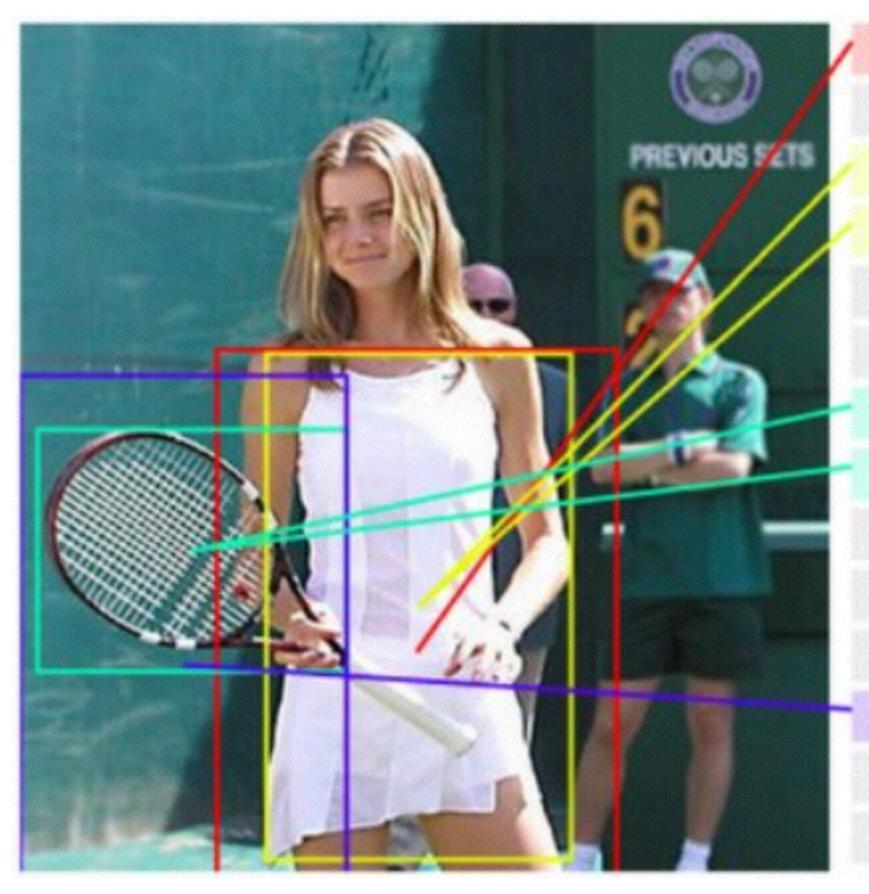


Human: Three different types of pizza on top of a stove.

Model sample 1: Two pizzas sitting on top of a stove top oven.

Model sample 2: A pizza sitting on top of a pan on top of a stove.





1.12 woman

-0.28 in

1.23 white

1.45 dress

0.06 standing

-0.13 with

3.58 tennis

1.81 racket

0.06 two

0.05 people

-0.14 in

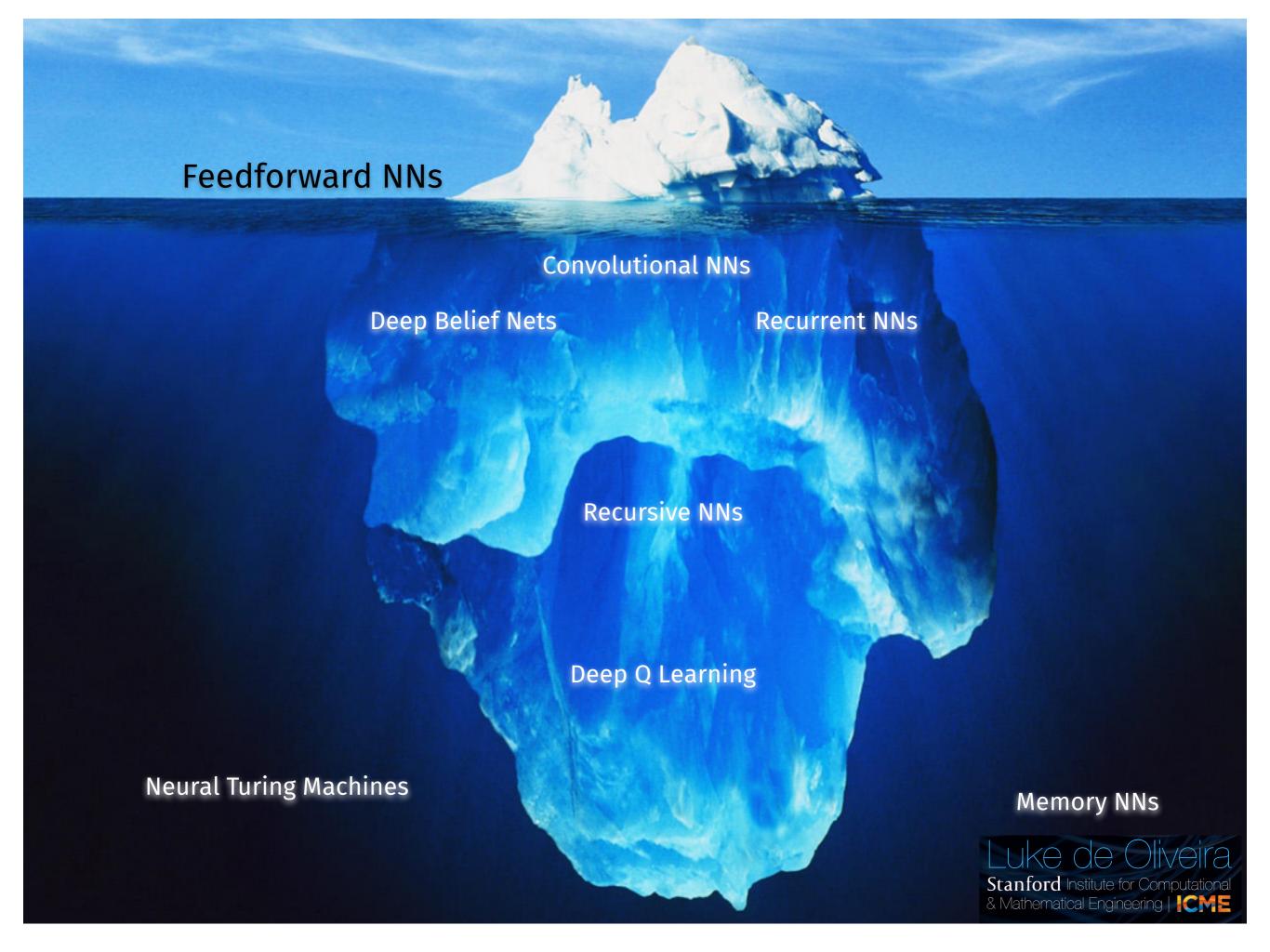
0.30 green

-0.09 behind

-0.14 her

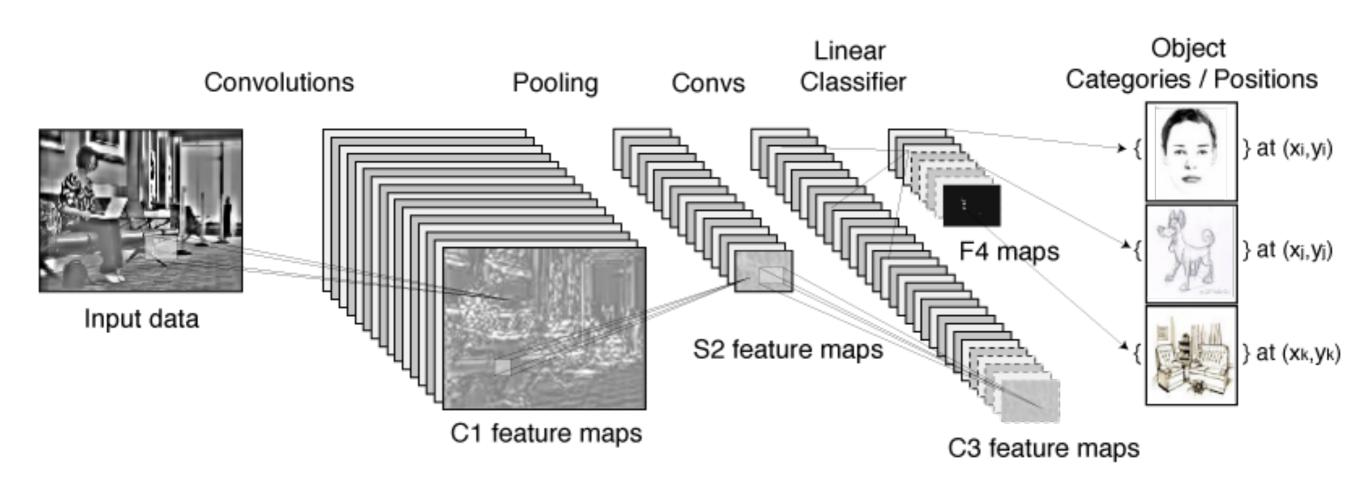
DNN Basics

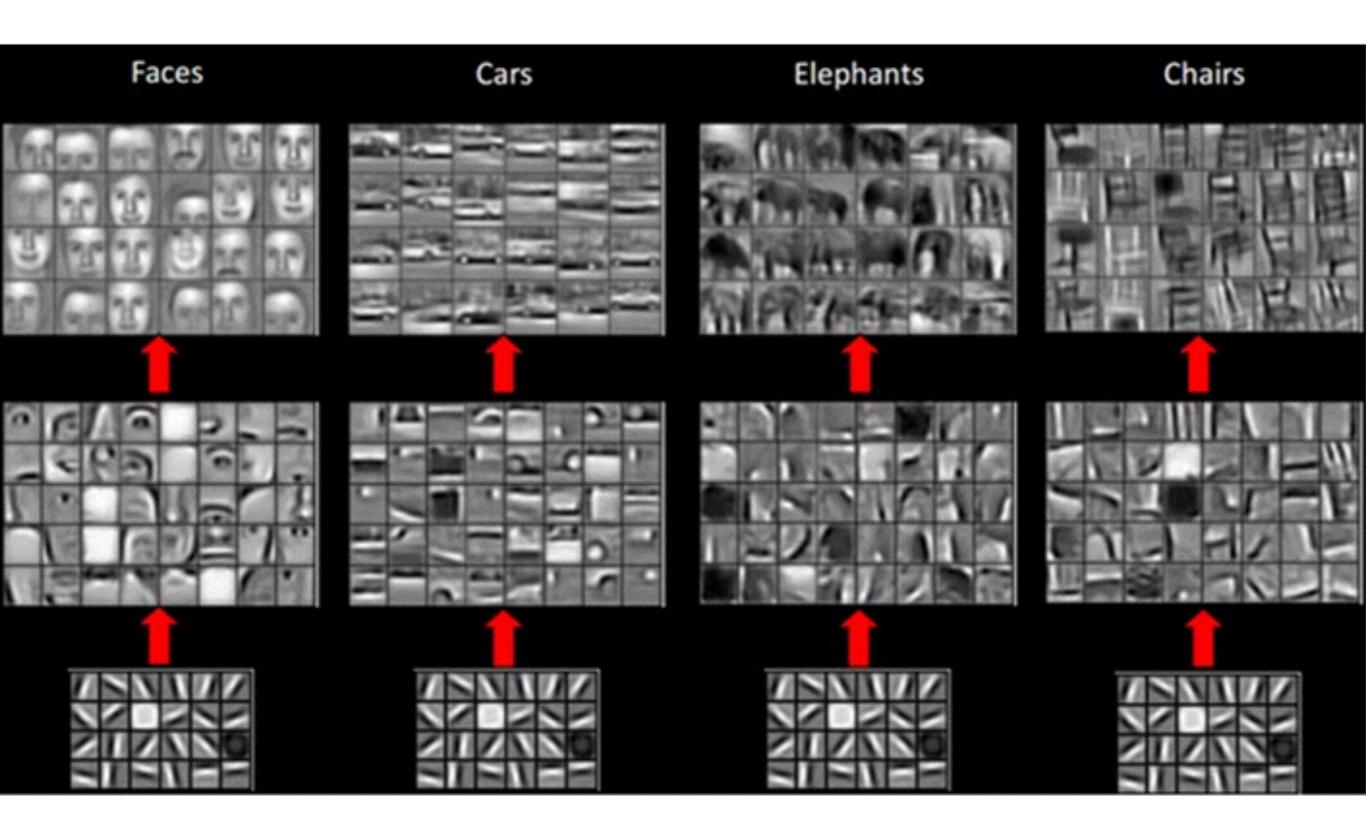
- 2 Primary Classes of problems:
 - Classification
 - Regression
- 2 Classes of inputs:
 - Fix size input
 - Variable size inputs (typical solution: Recurrent NNs)
- Learning Approaches
 - Supervised: labeled data
 - Unsupervised: unable data
 - Reinforcement training: try, succeed/fail?
- Representational networks: build an internal representation of input/output
- NNs can encapsulate arbitrary functions.



Convolutional NN

• 1D: Time series, 2D: images, 3D: video



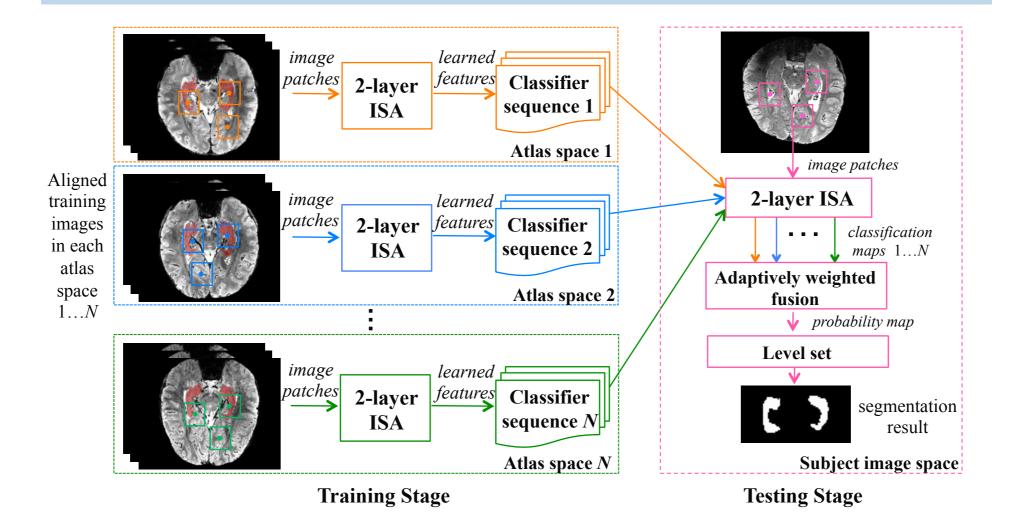


DNN in Medical Imaging

- Don't know much about it, but quick googling shows lots of examples
- Demonstrated for a variety of tasks
 - Mapping from image to Atlas
 - Measuring properties of regions (e.g. size of brain region)
 - Diagnosis (e.g. Alzheimer's Disease)
 - And more

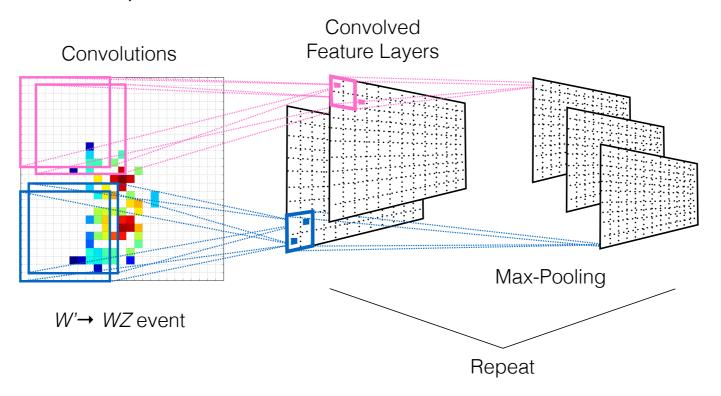
Multi-Atlas Segmentation





HEP and DNN

- Daniel Whiteson et al showed that (<u>NatureCom</u>, <u>Archive</u>)
 - DNN can work better than other techniques for sig/bkg rejection for searches.
 - DNNs can reproduce physics features (e.g. masses) from four vectors.
- Proof that DNNs use "Renormalization" to recognize cats (Wired)
- SLAC group is classifying jets and analyzing jet substructure (Slides)
- I know of others... but through private conversations...
- Seminar at Fermilab tomorrow on DNN in Nova (by Adam Aurisano)
- DNN & LArTPC? Seems like a perfect match.



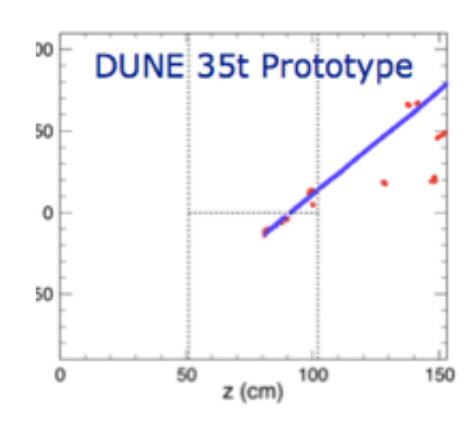
DNN Reco

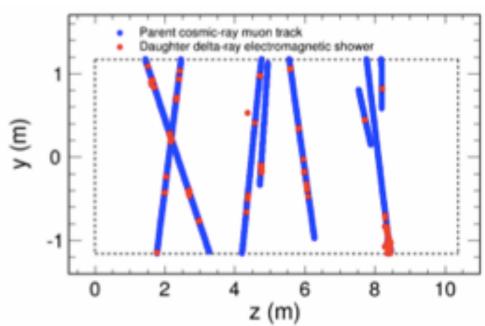
Motivations?

- Hopefully DNN-based feature extractors out perform hand crafted reconstruction algorithms.
- After training, DNN-based will likely to be much faster than algorithmic reconstruction.
 And it's already running on GPUs.
- There is incredible value (CHF/dollars) in the fact that DNN may allow performing reconstruction without physicists writing algorithms.
- For LArTPC, it may be able to do something we cannot do algorithmically.
- Maybe instead of writing reconstruction software, new workflow:
 - Train DNN on Simulated Data, perhaps starting with simplified training samples and work towards full complexity. Try different NNs, search hyper-parameters, ...
 - Calibrate with the full standard simulation samples of the experiment.
 - If some sub-class of events not are well "reco'd", add addition training sample. Iterate.
 - Apply to data, perhaps compare to hand scan and use re-enforcement training.

CNN for LArTPC

- My first attempt: DUNE-35 ton
- Goal: classify raw data: Stopped muons, radiated photons, horizontal cosmics, ... are small but very useful subset of data.
- How do we make samples of these w/o full reconstruction?
- I faked some events passing/stopped muon events, fed it to NVidias DIGITS, which is a DNN image classification tool.
 - Really just a very simple proof of principle test.





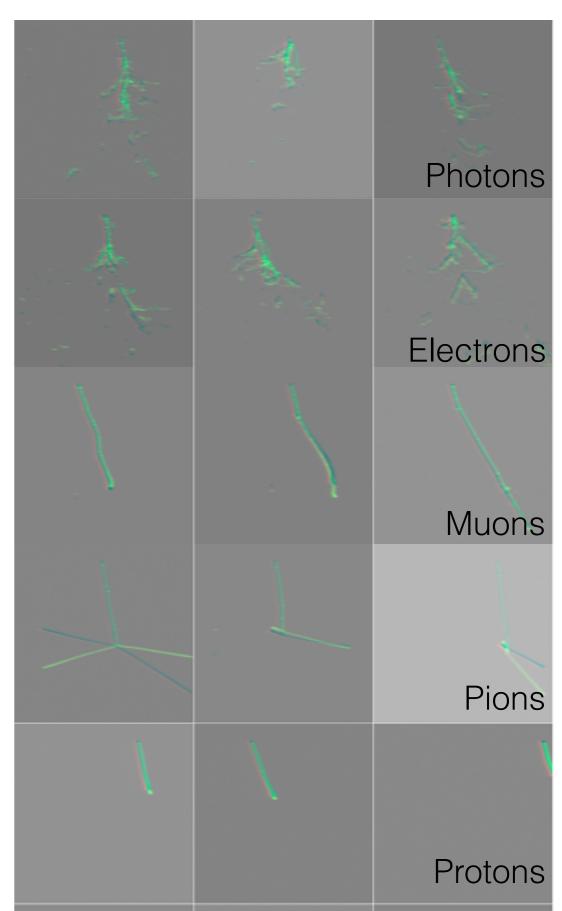
DNN Classification of "Raw" LArTPC Data

GoogleLeNet 256x256 Passing Stopped

1-4 Tracks With or without noise, DNN correctly classifies ~90-99%

Particle ID in LArIAT

- Another proof of principle test with lots of obvious things to fix.
- LArIAT is a small detector: 2 wire places with 240 wires each, 4096 samples.
- Generated single 500 +/- 200 MeV particles. 50k of each type.
- Used standard implementation of GoogLeNet, which takes 224x224 pixel color images (png files!).
 - Suspect that png conversion + image whitening causes loss of charge "scale".
 - I realized late that it was converting 240x256 to 224x224.
- Reduced samples by
 - Down sample: Summing N ticks, where N=1-8.
 - Scanning for the box with maximum total charge.
 - 2 planes -> R and G color intensities.
- Very preliminary... not completely understood.



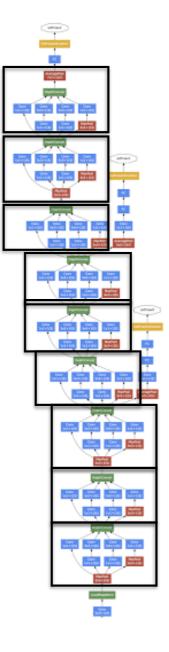
GoogLeNet

2014-era Model for Object Recognition



Module with 6 separate convolutional layers

24 layers deep!



Developed by team of Google Researchers:

Won 2014 ImageNet challenge with 6.66% top-5 error rate

http://arxiv.org/abs/1409.4842

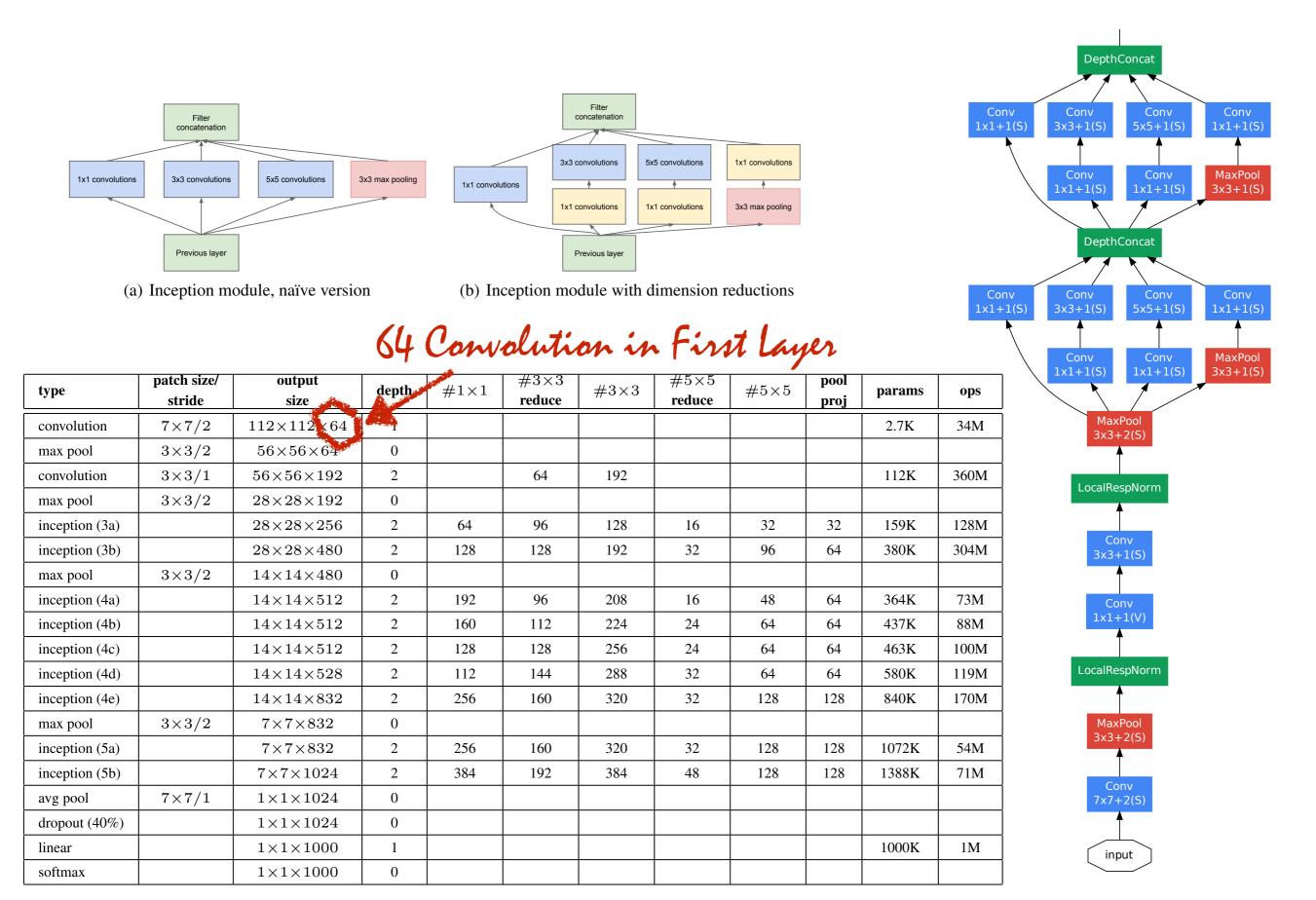
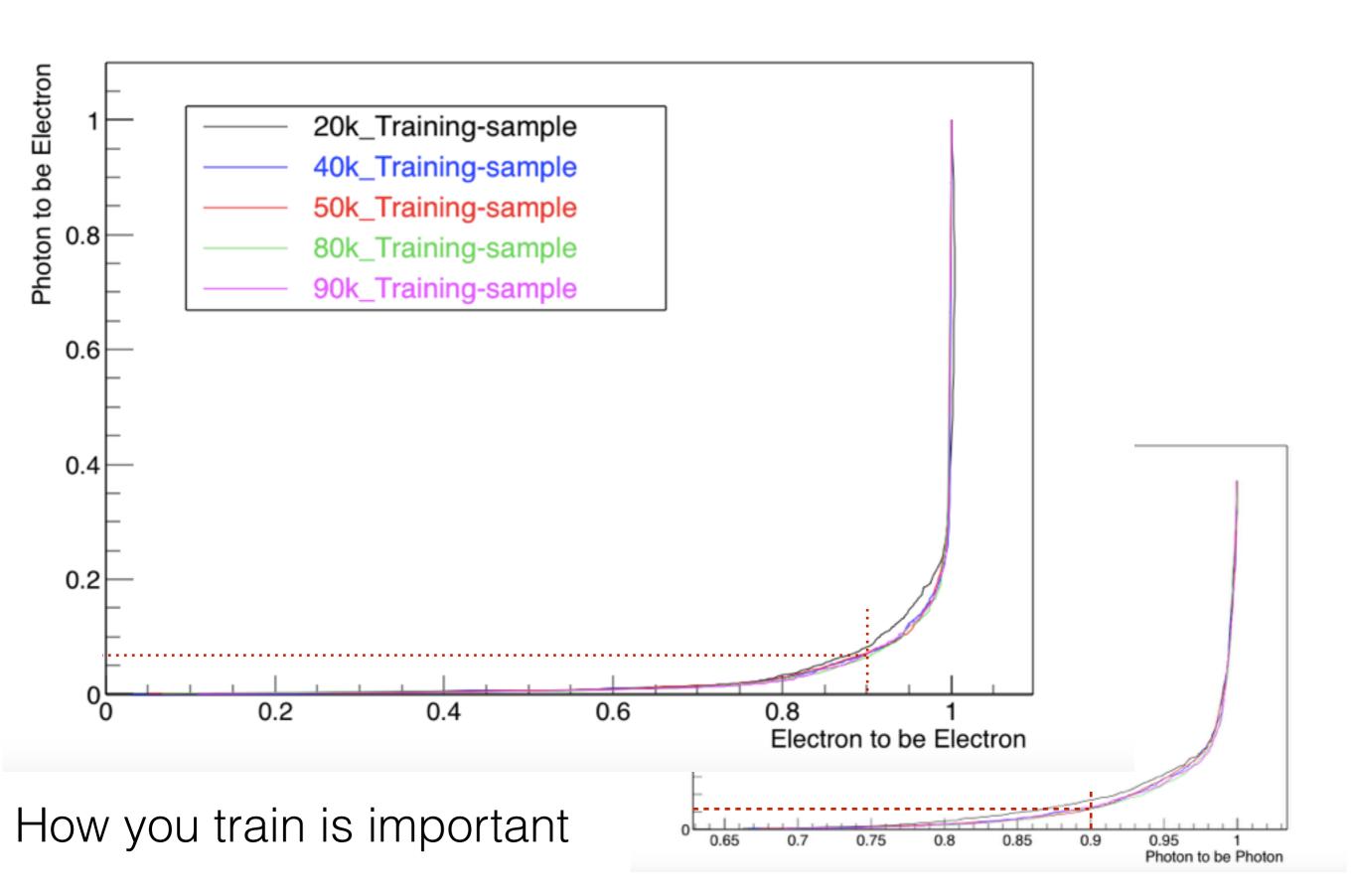
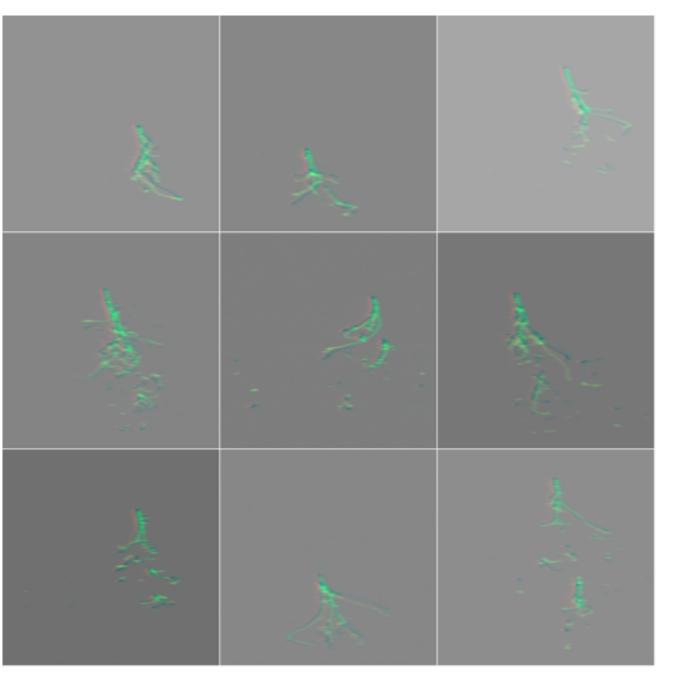


Table 1: GoogLeNet incarnation of the Inception architecture

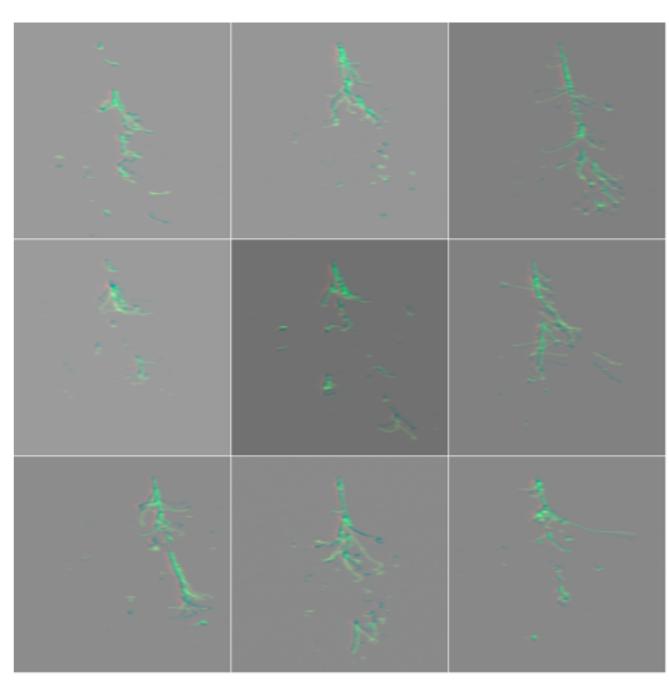
Electron vs Photon



Electron vs Photon

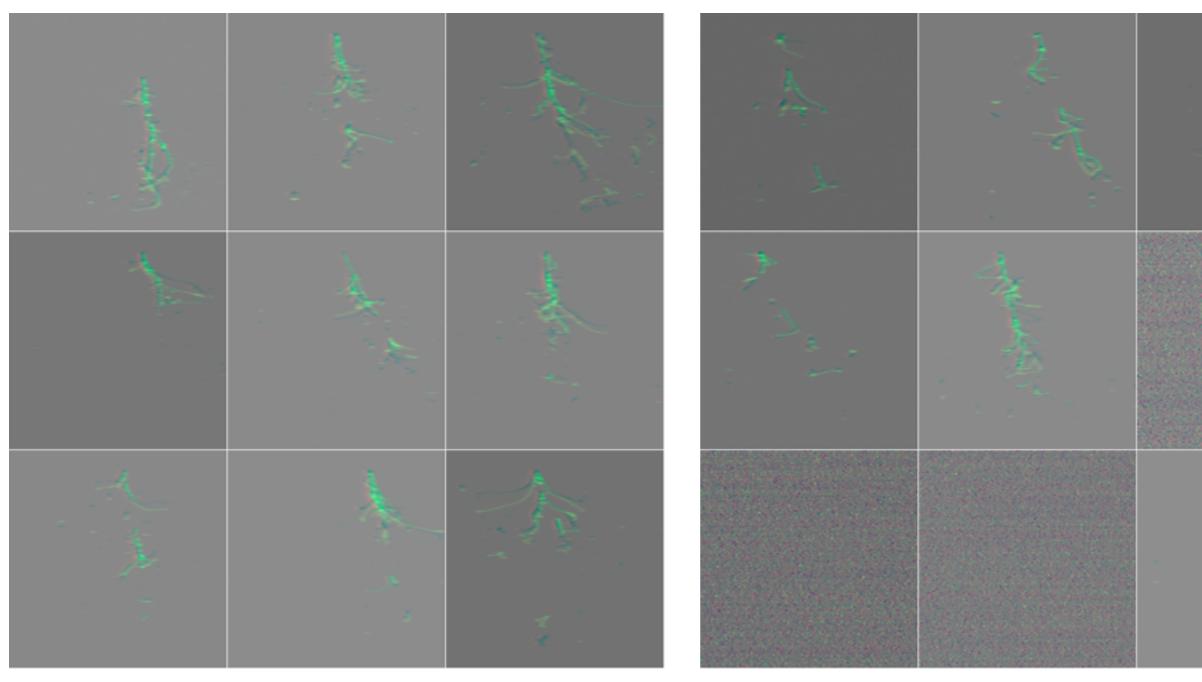


Real Photons ID as Photons



Real Electrons ID as Electrons

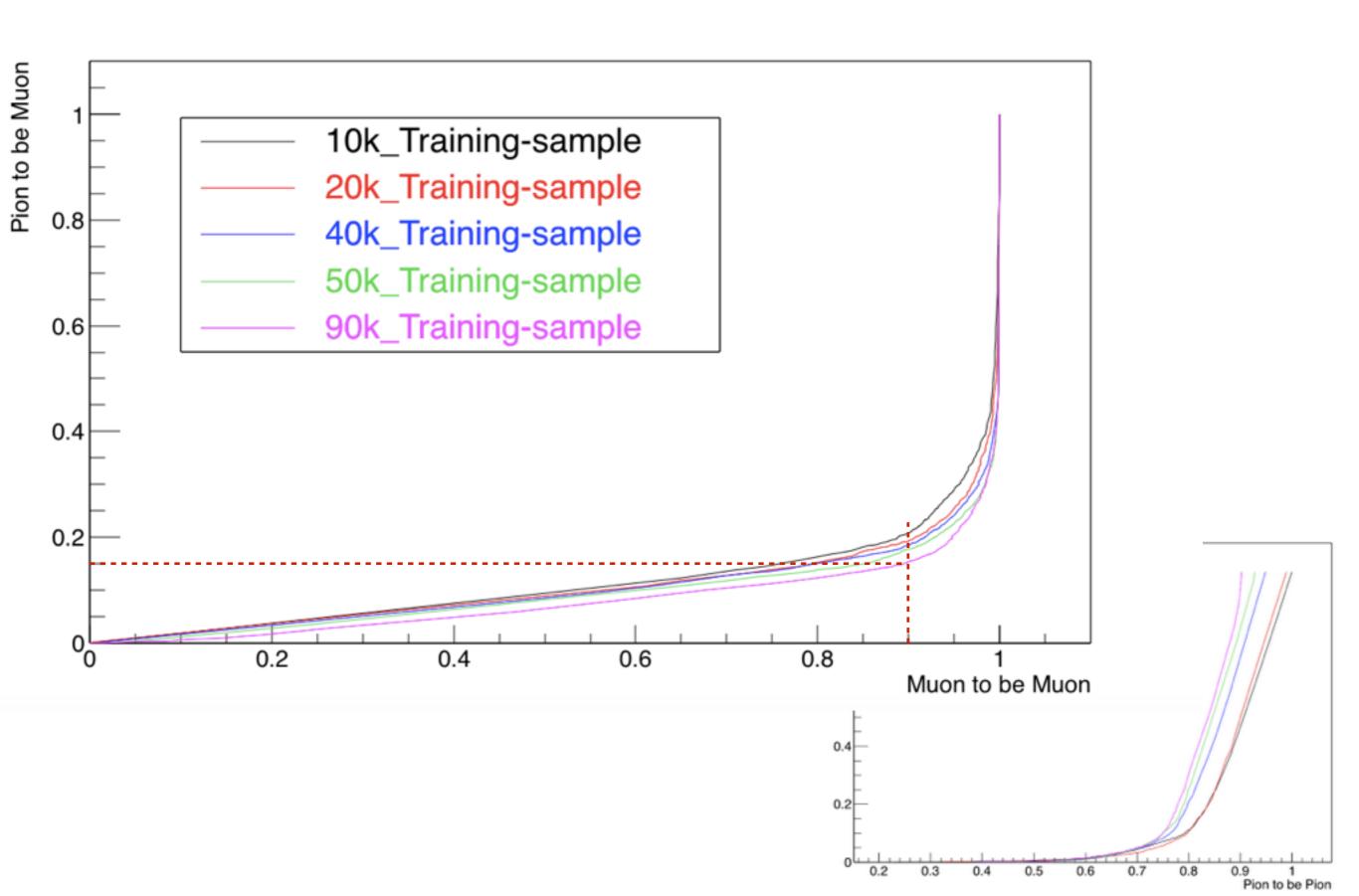
Electron vs Photon



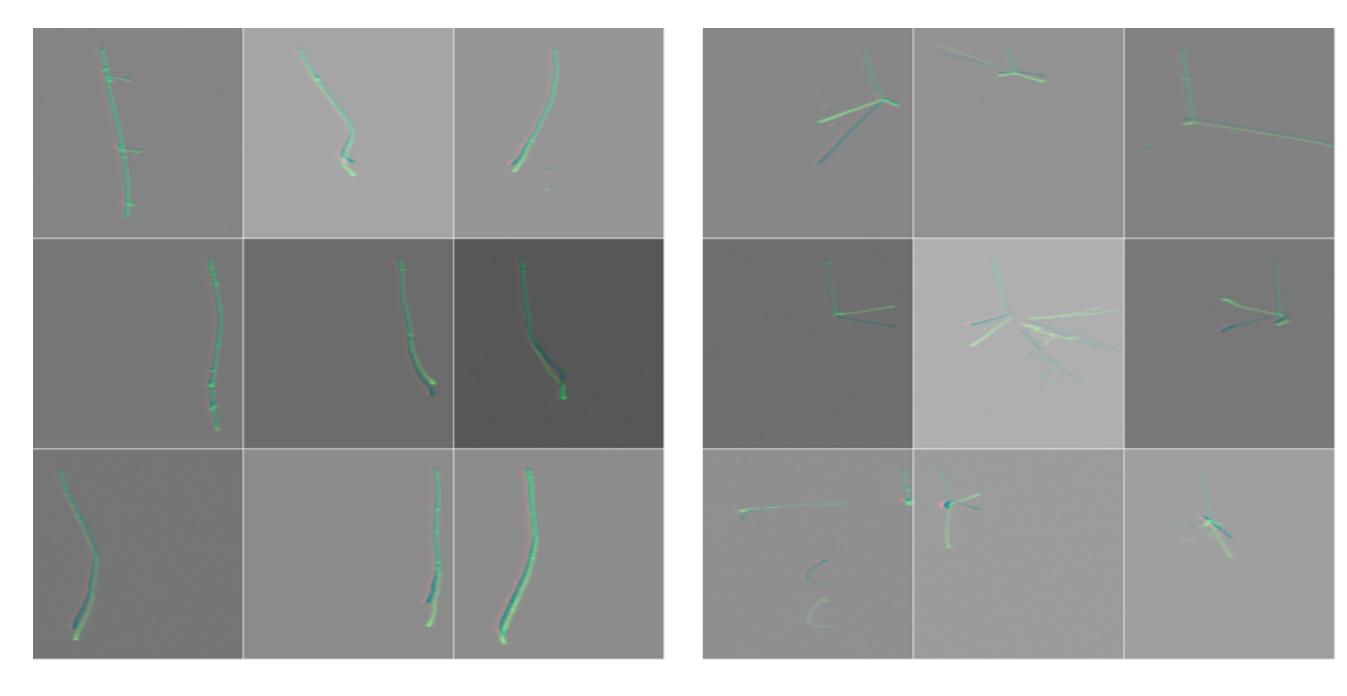
Real Electrons ID as Photons

Real Photons ID as Electrons

Muon vs Pion



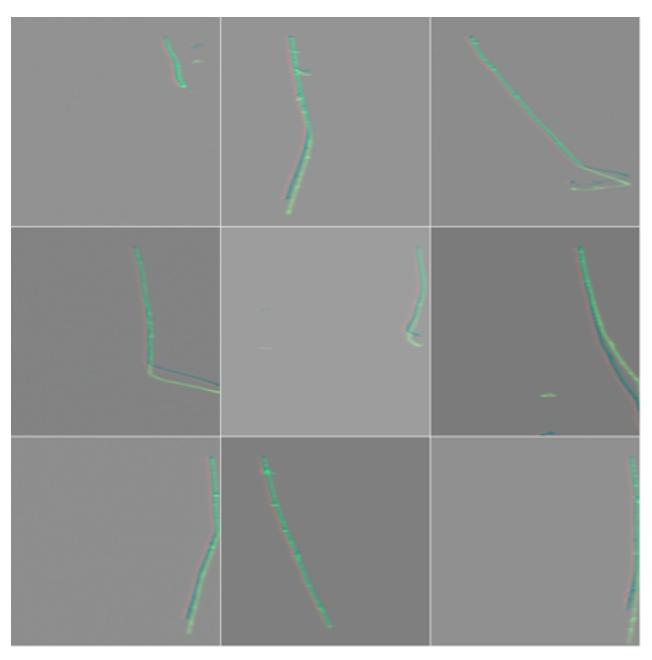
Muon vs Pion



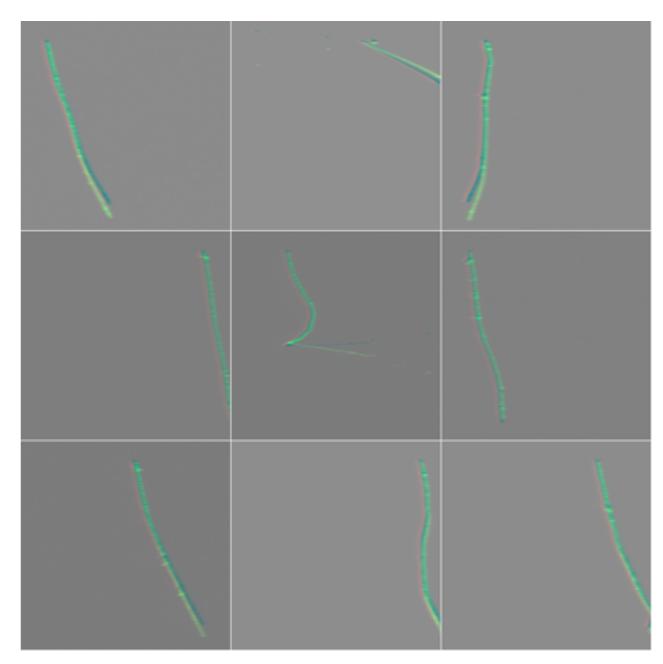
Real Muons ID as Muons

Real Pions ID as Pions

Muon vs Pion

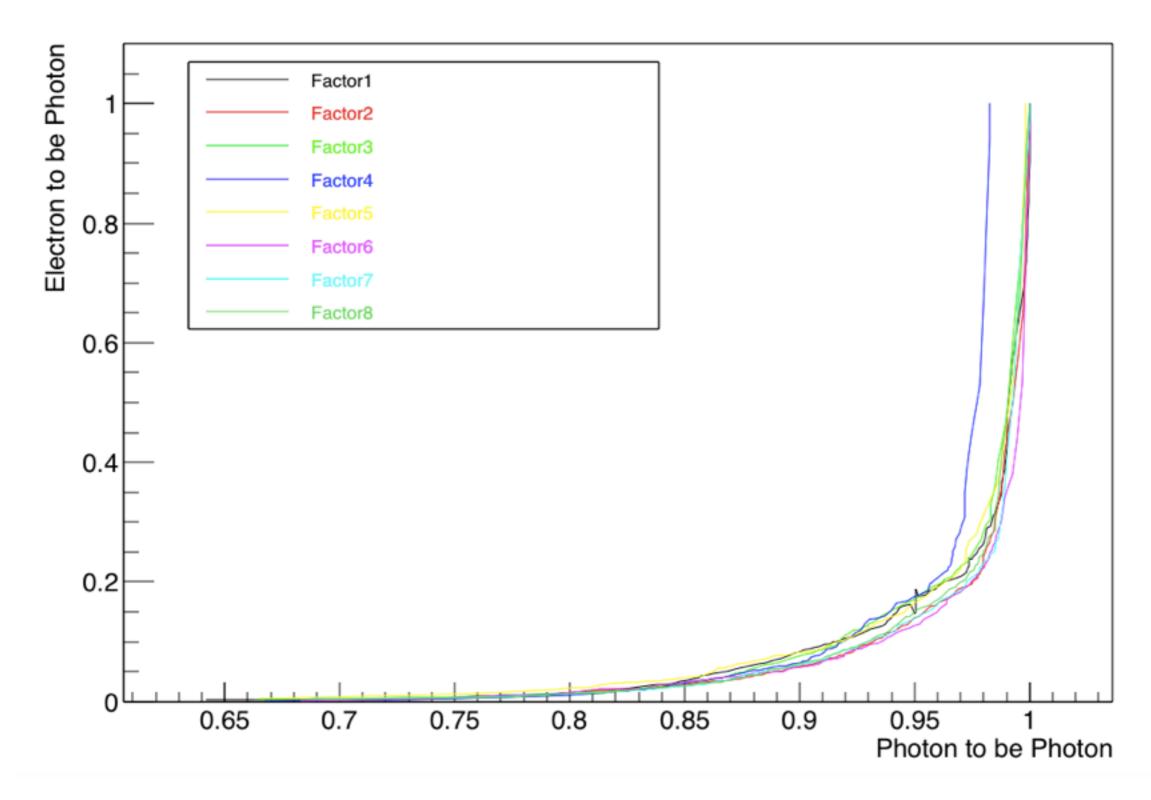


Real Muons ID as Pion



Real Pions ID as Muon

Down Sampling

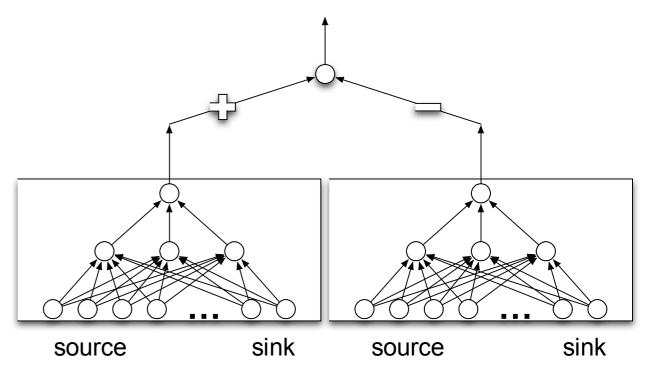


Competition between resolution vs capturing whole interaction

Next Steps

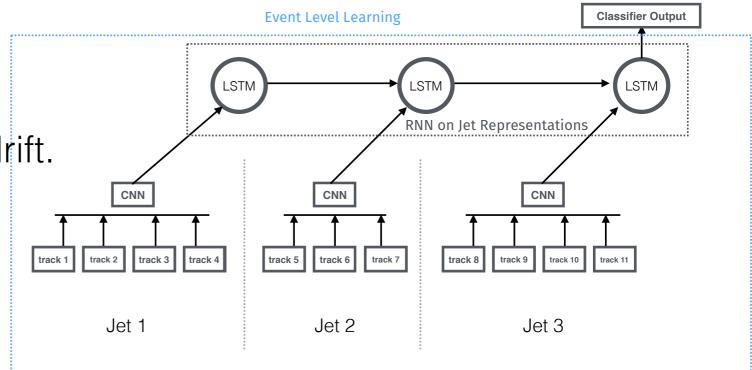
- Add neutrinos... currently I'm classifying whole events.
- Start modifying GoogLeNet.
- Just started collaboration with P. Baldi and P. Sadowski from UCI
- First task: how do we properly feed in the different views?
 - Their suggestion: Siamese NN
 - Perhaps we could train a network to resolve the ambiguities (1D x 1D => 2D), similar to WireCell?
 - Need to provide true hit info
 - Perhaps 2D x 2D => 3D, to take advantage of "connectivity" and topology.
- How much down sampling?
- What is appropriate size of convolutions? Hyperparameter optimization.
- Adding regression to estimate the energy should be straight forward.

Siamese Architecture



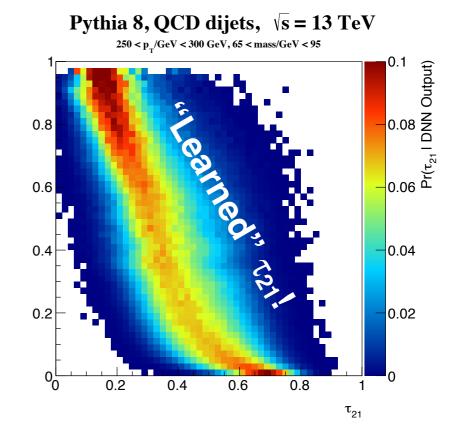
Improving Performance

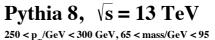
- Identify misclassified events
 - additional training on sample of such events.
 - add new classes to better separate them.
- Create classes based on final state content and topology.
 - Need to come up with some classification based on truth.
- Use Region-CNNs to identify regions with individual particles in multi-particle events.
 - Remove cosmics.
 - Feed to RNNs to classify full drift.

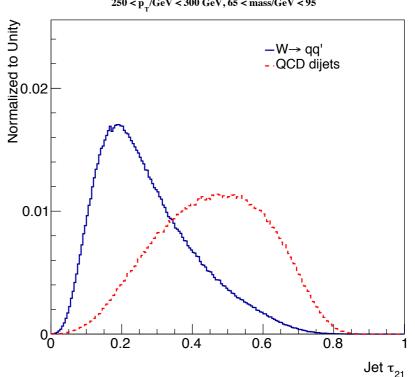


Inside the Black Box

- Studying DNNs can reveal useful features which we don't know about.
 - SLAC group got insight into colorflow!
- Look for correlations between DNN output and known features
 - Did the DNN figure out this feature?
 - How important is this feature?





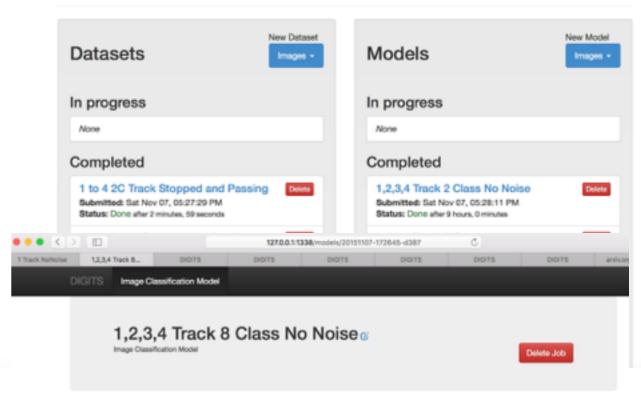


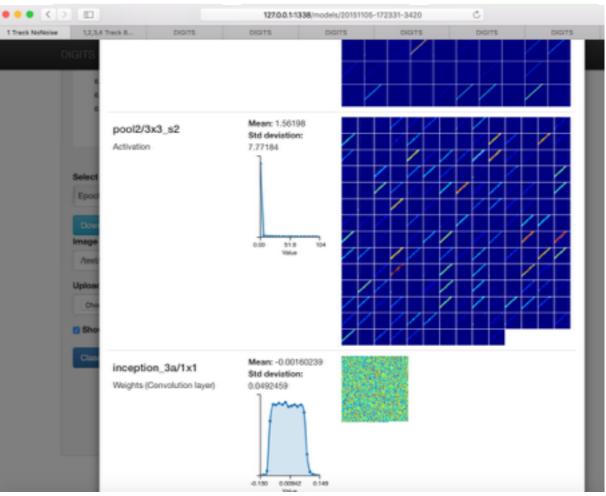
DIGITS

- Great way to play.
- Essentially a web server interface to a batch system. Multi-GPU support.
- Only image classification (for now?).
- Great potential of evolving to more a general tool that will also make DNN accessible to everyone.
 - A graphical model editor would be awesome.



Home





DAG-Based Frameworks

Processor Landscape

- Parallelism taking off:
 - Multi-core CPUs, with built in GPUs.
 - Many-core GPU/MiCs
 - OpenCL Programmable FPGAs (and ASIC?)
 - Potential to easily move algorithms from software to hardware.
 - On the horizon:
 - CPU/GPU/RAM Stacking
 - CPU+FPGA on same Dye
 - Neuromorphic Chips

HEP Software Landscape

- Shift from Fortan to C++ in late 1990s.
- The biggest datasets until mid 2000s... industry now leads.
- Problems:
 - Extremely complicated C++ frameworks, data structures, ...
 - Difficulty utilizing Multi-core CPUs and massively parallel GPU/MiC co-processors... or any future emerging technology.
 - Expensive: ATLAS software cost ~O(250 Million) CHF to build over 15 years...
 - starting from scratch (to deal with Parallelization problems) for Run 3 wasn't an option for ATLAS or CMS.
 - We cannot find developers to fill mission critical posts. Critical people get stuck in jobs...
 - We do not educate HEP PhDs in software... rely on talented people training themselves.
 - There is a culture that software isn't physics... but electronics and hardware are!
 - e.g. we do not support software R&D.

Parallelization Problem

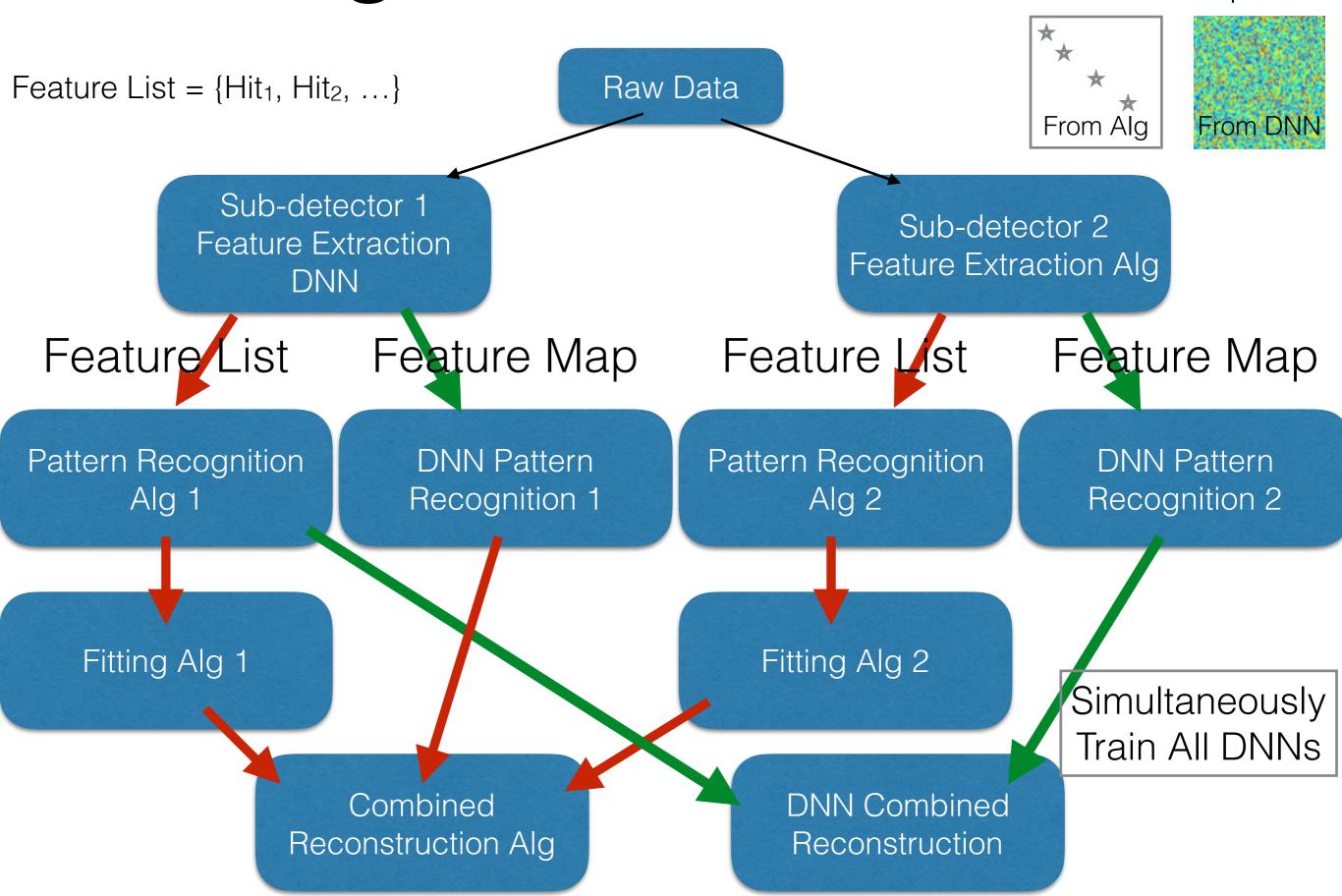
- Multi-core CPUs: we are quickly approaching 100's of cores/CPU.
 - Currently relying on Embarrassingly Parallel nature of HEP data.
 - Filling CPU cores with independent instances of software.
 - Not practical to have 4 GB/core for 100's of cores...
 - Not enough bandwidth to memory if every core needs to access different 4 GB.
 - C++ data structures make it difficult to take advantage of vectorization.
- Many-core Co-processors (possibly within CPU dye): GPUs/MiCs, FPGA, (ASICs?)
 - Requires *Data Parallelization* where (for example) many events are simultaneously processed in each algorithm. HEP frameworks designed to see 1 event at a time.
 - Difficult to code. Highly sensitive to optimization and hardware. Difficult to efficiently integrate with current software. Rapidly evolving ecosystem.
 - Mostly used in specialized systems like DAQ and Trigger. No good solution for offline.

HEP SW Wish List

- Reconstruction closely integrating:
 - Traditional Algorithms like ones in HEP SW today.
 - Deep Neural Networks (and other ML Techniques)
 - Automatic training/monitoring (e.g. for reproducing training in every release)
 - NN visualization (structure and weights), Hyper-parameter scans.
 - Image processing algorithms
 - Event Display / Hand Scan (e.g. for re-enforcement training)
- Data structures optimized for architecture and computation, with automatic data transformations.
- Algorithms can process many events at once.
- Automatically optimized for all/any CPU or GPU architectures. Future proof.
- Allow physicists to focus on the method and performance not implementation.
 - Easier to hand off problem to professional programmers.

Weaving-in DNN Reco

Feature Map =



Looking Ahead...

- Concurrency (simultaneously processing many events) is a hot topic. 2 types
 - Task Parallel: Many threads, each processing one event.
 - Data Parallel: Algorithms processing many events at once.
- The LHC experiments are confronting this issue. Current focus on Task Parallelism:
 - CMS already has multi-threaded ART.
 - ATLAS using plans to build on Gaudi-Hive for Run 3.
 - There are schemes to push some algs to co-processors... but not ideal.
- Experiments will have lifetime of decades (e.g. 30 years for DUNE). We need to insulate ourselves from architecture transitions.
- My opinion: We need new frameworks on the time-scale of HL-LHC, DUNE, ILC.
 - R&D Now. Framework in early 2020s. Reimplement software chain by 2025.

DNN Software

- Basic steps
 - Prepare data
 - Build Model
 - Define Cost/Loss Function
 - Run training (most commonly Gradient Decent)
 - Assess performance.
 - Run lots of experiments...
- 2 Classes of DNN Software: (Both build everything at runtime)
 - Hep-Framework-Like: e.g. Torch, Caffe, ...
 - C++ Layers (i.e. Algorithms) steered/configured via interpreted script:
 - General Computation Frameworks: Theano and TensorFlow
 - Everything build by building mathematical expression for Model, Loss, Training from primitive ops on Tensors
 - Symbolic derivatives for the Gradient Decent
 - Builds Directed Acyclic Graph of the computation, performs optimizations
 - Theano-based High-level tools make this look like HEP Frameworks (e.g. pylearn2, Lasagna, Keras, ...)

DNN Software

- Data is typically represented as numpy-like Tensors (N dim arrays).
 - Easily change between CPU and GPU implementations of tensor.
 - Usually automatically transferred between CPU/GPU memory.
 - Usually persistified in hdf5... sometimes stored in databases.
 - Supposedly very optimized.
- GPUs?
 - Most eventually call the same libraries (e.g. cuCNN) for optimized implementation.
 - Most have some library of algorithms with both CPU and GPU implementations.
 - Theano generates code for kernels and uses kernel libraries when appropriate.
 - Almost all on NVidia/CUDA... seeing OpenCL now.
 - I've seen significantly better performance from AMD over NVidia for some kernels.

Math in Python

- numpy: Matrix manipulation like matlab
 - C=A*B performs a computation on numbers in A and B matrixes
- sympy: Symbolic manipulation like mathematica
 - C=A*B; $D=A^{-1}C ==> D=B$
- Theano:
 - Symbolic representation and operations (e.g. derivatives)
 - Based on Tensors with numpy-like functionality
 - Computation tree optimization
 - Transparently compiles into CPU, OpenMP, CUDA, and OpenCL.
 - Many missing/non-optimal features in GPU implementation
 - Provides a framework for implementing new operations, optimizations, and backends.
 - Provides an environment built for optimizing calculations on CPUs and GPUs.
- Why? instead of writing code to perform you calculation, use these systems to write down the mathematical expressions... and they will generate *optimized* code.

Working with Theano

- Easy to switch from C to Python to Theano to Sympy, etc...
 - Just build your expression with python functions and feed the different objects for different versions.
 - consider: def f(x): x*x
 - python: y=f(2) -> y=4 (regular python float)
 - sympy: $y=f(x) \rightarrow y = symbolic rep$
 - theano: $y=f(x) \rightarrow y = symbolic rep$
 - compute_y=function([x],y) optimizes/compiles
 - compute_y(2) -> 4
- Various ways to convert sympy -> theano:
 - theano_function: takes a sympy expressions and translates it into Theano expression.
 - SymCFunc: creates efficient c-code for scaler expression which Theano can wrap...
 - The c-function can be faster.
 - But then Theano can't optimize it.
- Parallelization: tensor representation... numpy broadcasting for scaling.
- Loops = contraction of indexes... makes reordering loops easy
- Iteration = shared variables (keep state) and update mechanism.

MEM with Theano

- Matrix Element Method is in principle the most sensitive technique for searches, but has been prohibitively CPU intensive.
- Simple case (6 diagrams): u u -> 3 gamma matrix element. One of the first examples of ME on GPU from 2010. (based on http://arxiv.org/pdf/
 0908.4403.pdf)
 - Note interesting LHC processes have O(100) diagrams.
- Focusing on ME evaluations only... no integration, change of vars, etc...
- I count ~ 500 real and 500 complex numerical operations in the ME calculation (~1500 total).
 - c-code → python → Theano reduces operations to ~1000.
 - c-code → python → sympy → Theano reduces the operations to 321 (116 on GPU, but I can't compile!)
 - 5.1x (4.6x) faster per event single thread computation time float (double).

Theano

- Might be trivial to implement some algorithms with Theano.
 - Anything you can write as a formula can be easily expressed in Theano and automatically optimized.
 - Many things are already implemented.
 - For example, Kalman Filter (from: http://matthewrocklin.com/blog/work/2013/04/05/
 SymPy-Theano-part-3/

```
from sympy import MatrixSymbol, latex
                                     # Number of variables in our system/current stat
       = 1000
       = 500
                                     # Number of variables in the observation
       = MatrixSymbol('mu', n, 1) # Mean of current state
Sigma = MatrixSymbol('Sigma', n, n) # Covariance of current state
       = MatrixSymbol('H', k, n) # A measurement operator on current state
       = MatrixSymbol('R', k, k) # Covariance of measurement noise
       = MatrixSymbol('data', k, 1)
data
                                     # Observed measurement data
       = mu + Sigma*H.T * (R + H*Sigma*H.T).I * (H*mu - data)
                                                               # Updated mean
newSigma= Sigma - Sigma*H.T * (R + H*Sigma*H.T).I * H * Sigma
                                                               # Updated covariance
inputs = [mu, Sigma, H, R, data]
outputs = [newmu, newSigma]
dtypes = {inp: 'float64' for inp in inputs}
from sympy.printing.theanocode import theano_function
f = theano_function(inputs, outputs, dtypes=dtypes)
import numpy
ninputs = [numpy.random.rand(*i.shape).astype('float64') for i in inputs]
nmu, nSigma = f(*ninputs)
```

DAG Framework?

- Today with Theano
 - A Physicists can write down math expression for their computation or algorithm.
 Theano auto optimizes...
 - no computing expertise necessary.
 - Can pass expression to professionals who tune optimization/code generation in Theano
 - No physics understanding necessary.
 - Code generation can be optimized for each architecture.
- Naively, we should consider completely different approach to writing software:
 - High level description of algorithms/data by physicists (new language?)
 - The representation of the data and the implementation of the computation is changeable.
 - Automatic analysis of the computation graph and targeted code generation, developed/optimized by experts

TensorFlow

- Google Deep Learning tool, many similarities to Theano, recently open sourced. C++ and python API.
 - Computation is done by building a DAG in a Session. Performs DAG optimizations.
 - Library of operations which wrap CPU and GPU kernels
 - Extendable.
 - Ops can provide gradient implementation.
 - Doesn't generate code like Theano.
 - Provides control flow operations which allows implementing loops.
 - Variables provide mutable data.
 - Containers allow sharing mutable data between disjoint computation graphs.
 - Queues automatically provide asynchronous computation when possible.
 - Designed for heterogeneous and distributed computing.
 - Point is that the same code generate same computation on any system.
 - From mobile phones, to multi-gpu systems, to heterogeneous distributed clusters.
 - Optimizes kernel placement using cost models, simulations, measurements of performance of kernels on devices and data transfer times.
 - Has Fault Tolerance.
 - TensorBoard provides graph and data visualization.

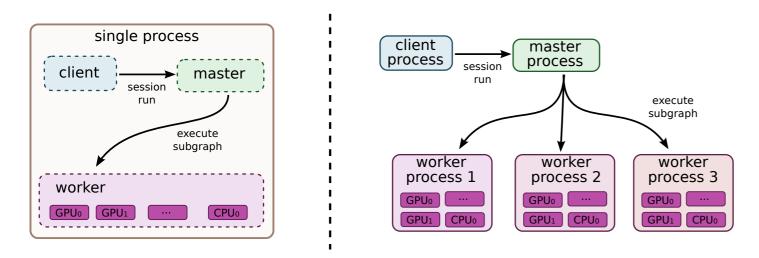


Figure 3: Single machine and distributed system structure

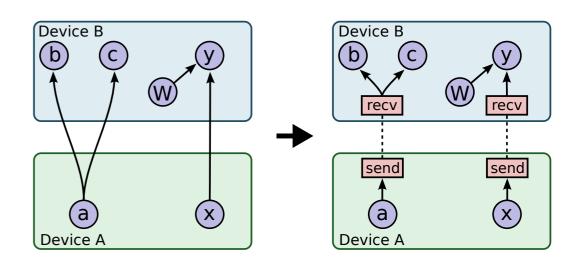


Figure 4: Before & after insertion of Send/Receive nodes

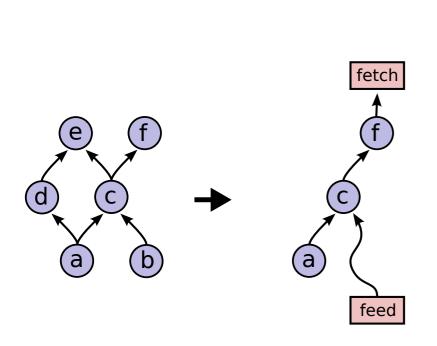


Figure 6: Before and after graph transformation for partial execution

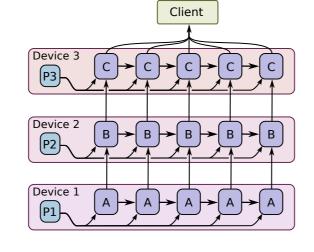


Figure 8: Model parallel training

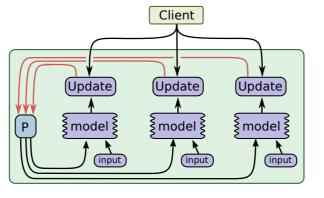


Figure 9: Concurrent steps

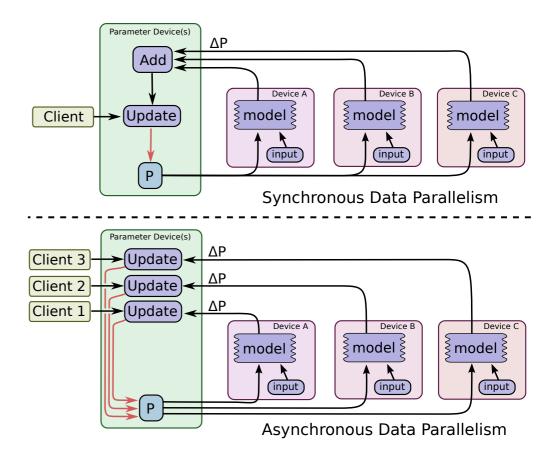


Figure 7: Synchronous and asynchronous data parallel training

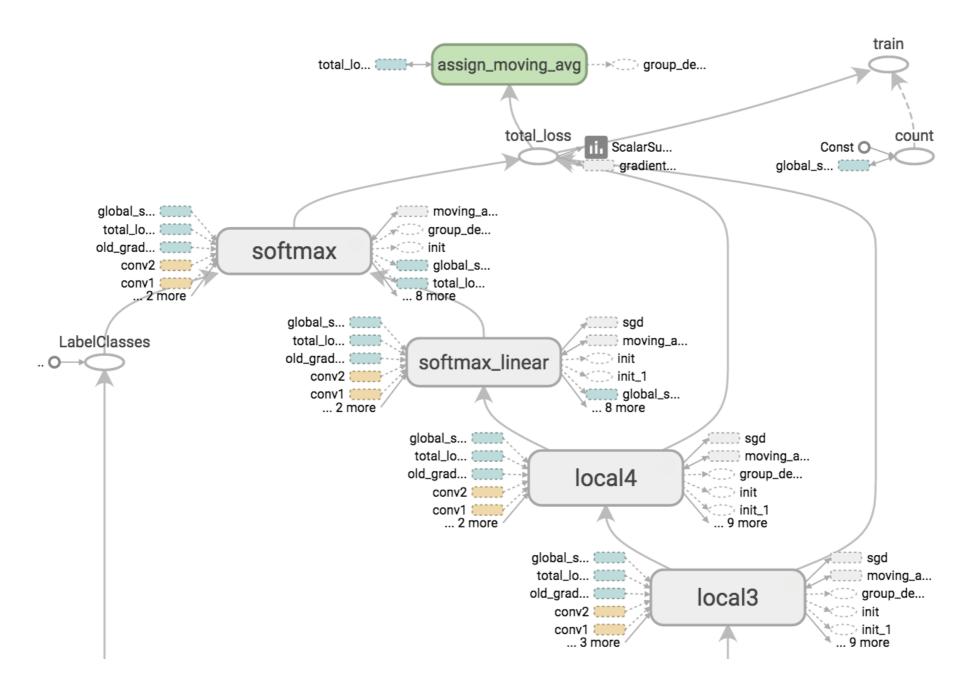


Figure 10: TensorBoard graph visualization of a convolutional neural network model

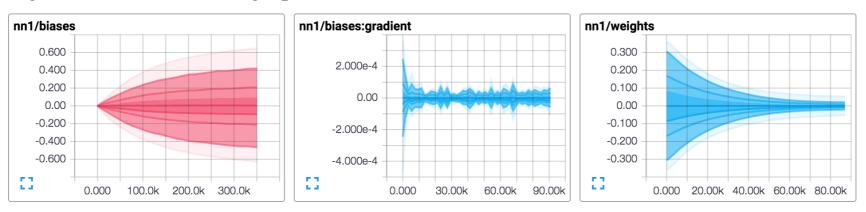


Figure 11: TensorBoard graphical display of model summary statistics time series data

DAG/Tensor Based Systems

- TensorFlow paper points out that there are many other similar systems
 - None provide the level of support for heterogeneous and distributed systems.
 - Few have features that TensorFlow intends to implement.
 - For example automatically generating kernels that more efficient by combining operations.
- Clearly there is a some of commonality with Gaudi-Hive, WireCell 2.0, etc...
- The appeal of TensorFlow is that it will be supported by Google and open source community.
 - Potential to outsource the low level details and optimization to Google, community, and non HEP-professionals.
- If not the basis, these systems may provide inspiration for future framework.

DAG/Tensor HEP Framework?

- I can imagine building Reconstruction, DAQ, or Trigger based on this system.
- Reconstruction our extremely complicated...
 - Some steps (e.g. FFT deconvolution) could be implement in a few lines using existing ops.
 - Complex algorithms can be written into Ops/Kernels.
 - These can be wrapped by an abstractions analogous to ART Modules/Gaudi Algorithms.
 - Similar to high level DNN SW build on top of Theano.
- Our Data is complicated
 - Representation as tensors is efficient for vectorization, GPUs, and easily segmenting data.
 - · High Level Objects can wrap these objects.
 - Not sure Event Store is necessary in Data Flow approach... could be faked (e.g. simple python dictionary)
 - Data isn't fetched at run-time.
- Not sure how to handle Conditions Database, Geometry, etc...
- I think implementing WireCell in TensorFlow or Theano is perfect R&D for such an idea.

Final Thoughts

- LArTPC is ideally suited for Deep Learning
 - Minimally, we could provide better classifiers based on engineered features.
 - Classification based on raw data is analogous to the impressive CNN image recognition already demonstrated.
 - My extremely simple study is very promising.
 - Measuring energy seems like straight forward extension.
 - Classification + energy is all we need for neutrino physics, right?
 - R-CNNs can extend this approach to busy events.
 - Not clear if best to look at event as a whole or reco events particle by particle.
 - We could also consider DNNs that perform specific parts of our standard reconstruction, perhaps the ambiguity resolution of WireCell?
 - Hand scans and Reinforcement training seem like a perfect fit.
- I believe future frameworks will have many features already in DNN SW like TensorFlow
 - Minimally, we should learn from these systems.
- Building our frameworks on top of a broadly used system is highly desirable.
 - Save a lot of time/manpower/money.
 - Allow physicists to focus on physics. Easy to try ideas. Let "professionals" worry about the hard technical stuff.
 - Provide access to broader range of architectures and resources... future-proof.